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Novel Algorithms/High Performance Computing Arising in Molecular Electronic Structure Theory

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Deadline for manuscript submissions:
closed (30 June 2019)

Message from the Guest Editors

Dear Colleagues,

This Special Issue will consist of manuscripts describing recent advances in the understanding and prediction of the electronic structures of molecules. Many of these advances are concurrent with the development of new algorithms and deployment of existing algorithms on new architecture. Manuscripts that describe new methods for strong correlation in molecules (or molecular fragments) that avoid the steep factorial scaling of fully variational methods are particularly encouraged (e.g., stochastic models). The Special Issue is expected to include submissions on molecular properties, including relativistic effects and the practicable inclusion of quantum electrodynamics (QED). Many of the new developments make extensive use of GPUs and other architectural advances in computers.

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Message from the Editor-in-Chief

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